SENSITIVITY AND UNCERTAINTY ANALYSES OF CROP YIELDS AND SOIL ORGANIC CARBON SIMULATED WITH EPIC

X. Wang, X. He, J. R. Williams, R. C. Izaurralde, J. D. Atwood

ABSTRACT. *Modeling biophysical processes is a complex endeavor because of large data requirements and uncertainty in model parameters. Model predictions should incorporate, when possible, analyses of their uncertainty and sensitivity. The study incorporated uncertainty analysis on EPIC (Environmental Policy Impact Calculator) predictions of corn (*Zea mays *L.) yield and soil organic carbon (SOC) using generalized likelihood uncertainty estimation (GLUE). An automatic parameter optimization procedure was developed at the conclusion of sensitivity analysis, which was conducted using the extended Fourier amplitude sensitivity test (FAST). The analyses were based on an experimental field under 34-year continuous corn with five N treatments at the Arlington Agricultural Research Station in Wisconsin. The observed average annual yields per treatment during 1958 to 1991 fell well within the 90% confidence interval (CI) of the annually averaged predictions. The width of the 90% CI bands of predicted average yields ranged from 0.31 to 1.6 Mg ha^{-1}. The predicted means per treatment over simulations were 3.26 to 6.37 Mg ha^{-1}, with observations from 3.28 to 6.4 Mg ha^{-1}. The predicted means of yearly yield over simulations were 1.77 to 9.22 Mg ha^{-1}, with observations from 1.35 to 10.22 Mg ha^{-1}. The 90% confidence width for predicted yearly SOC in the top 0.2 m soil was 285 to 625 g C m^{-2}, while predicted means were 5122 to 6564 g C m^{-2} and observations were 5645 to 6733 g C m^{-2}. The optimal parameter set identified through the automatic parameter optimization procedure gave an R^2 of 0.96 for average corn yield predictions and 0.89 for yearly SOC. EPIC was dependable, from a statistical point of view, in predicting average yield and SOC dynamics.*

Keywords. *Corn yield, EPIC model, GLUE procedure, Parameter optimization, Sensitivity analysis, Uncertainty analysis.*

Computer-based agronomic models are simplified representations of physical processes. The application of models generally involves large data requirements. Some of the input data and model parameters are not known with certainty, since they are often difficult to determine accurately due to the inherent variability in natural processes, costly monitoring, or imperfections in data measurements. Therefore, model predictions are not the absolute answers, and in most cases it may be preferable to give confidence interval estimates (Haan, 2002) rather than singular outputs due to uncertainties in both model structure and input values. It has been realized that identifying the probabilities of outputs with a quantitative uncertainty analysis and evaluating their likelihood can provide decision/policy makers with more valuable information to make or evaluate decisions (Haan and Skaggs, 2003a; Ogle et al., 2003). Sensitivity analyses can help in inspecting the main sources of model prediction uncertainty. It helps identify the critical control points, prioritize additional data collection or necessary research, and select calibration parameters. Therefore, good modeling practice requires the incorporation of uncertainty and sensitivity analyses (Haan et al., 1998; Hession et al., 1996; Reckhow, 1994).

Several methodologies have been used to account for uncertainty, such as Kalman filtering (Peter, 1979; Ahsam and O'Connor, 1994), first-order analysis (FOA) (Chaubey et al., 1999; Haan and Skaggs, 2003a, 2003b), Monte Carlo simulation (MCS) (Hession et al., 1996; Haan and Skaggs, 2003a, 2003b; Ogle et al., 2003), Latin hypercube sampling (LHS) (Pebesma and Heuvelink, 1999), and generalized likelihood uncertainty estimation (GLUE) (Beven and Binley, 1992; Beven, 1993). Among these methods, GLUE is a more comprehensive uncertainty analysis methodology based on MCS, likelihood measures, and the concept of Bayesian inference. It requires no assumptions of linearity, Gaussian approximation, or parameter independence. Parameter interactions and non-linearity in the model responses are handled implicitly in the GLUE methodology since the likelihood measure for each model realization is associated with a particular set of parameters rather than individual parameter values (Beven and Freer, 2001).

Sensitivity analysis methods can be classified as: (1) graphical methods, such as "visual" sensitivity analysis (Romanowicz et al., 1994); (2) mathematical methods; and (3) statistical methods, such as analysis of variance (ANOVA), response surface methods (RSM), and Fourier amplitude sensitivity test (FAST). Graphical methods can be used as a screening method before further analysis to give visual indication of how an output is affected by variation in inputs. Mathematical methods typically involve calculating the

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output for a few values of an input. These methods do not address the variance in the output due to the variance in the inputs. Statistical methods involve running simulations using inputs with given distributions and assessing the effect of variance in inputs on the outputs distribution (Andersson et al., 2000). These methods allow researchers to identify the effect of interactions among multiple inputs that vary simultaneously.

After sensitivity analysis, it would be worthwhile to get more information about the most influential parameters. It is common practice to calibrate those parameters to give the optimal fit to observations. Borah and Haan (1991) and Thorsen et al. (2001) stated that errors could be introduced into models during the calibration process due to imperfect data used for calibration, the chosen objective function and fitting criterion, and interaction of parameters. The calibration process can be done either manually, using a trial and error process of parameter adjustments, or by using computer-based automatic procedures. Madsen (2000) stated that it is possible for an experienced hydrologist to obtain very good and hydrologically sound parameters using manual calibration, but manual calibration is tedious, time-consuming, subjective, and cannot easily include consideration of the interaction among parameters. In computer-based automatic calibration, parameters can either be adjusted automatically through a specified optimization search algorithm or identified automatically among Monte Carlo simulations. Automatic calibration procedures have focused mainly on using a single overall objective function. However, a single performance measure is often inadequate to measure properly the simulation of all the important characteristics of the system that are reflected in the observations. This was what caused skepticism in the hydrological profession for applying automatic calibration procedures (Madsen, 2000). Recently, multi-objective function techniques have been applied in automatic calibration routines for rainfall-runoff modeling (Refsgaard, 1997; Madsen and Kristensen, 2002; Madsen, 2000; Gupta et al., 1998; Yapo et al., 1996).

The Environmental Policy Impact Calculator (EPIC) (Williams and Sharpley, 1989) is a continuous, field-scale agricultural management/water quality model. The major model components in EPIC are weather simulation, hydrology, erosion/sedimentation, nutrient cycling, pesticide fate, soil temperature, plant growth, tillage, and plant environmental control. It also calculates the cost associated with each modeled management practice. The model includes parameter data files for major crops, soils, fertilizers, and tillage practices. The most recent version, v3060, incorporates carbon and nitrogen algorithms to estimate soil carbon sequestration as affected by climatic conditions, soil properties, and management practices (Izaurralde et al., 2001a). Soil carbon sequestration is one technique with near-term potential for attenuating the rapid observed increase in atmospheric CO_2 (Izaurralde et al., 2001b). Models such as EPIC are being increasingly used to estimate soil carbon sequestration rates and overall potential at field and regional scales. The use of such models allows decisions to be made as to whether a particular management practice can result in soil carbon sequestration and whether the application of such practice is useful and cost effective, when field data, especially the necessary long-term data, are both difficult and expensive to obtain. While models could be well calibrated and perform adequately under many conditions, there is still uncertainty about the values of many of their parameters, which could add to the overall uncertainty in the outputs. In the case of EPIC, although it has been extensively tested and applied throughout the U.S. and many other countries (King et al., 1996; Pierson et al., 2001; Chung et al., 2002; Bernardos et al., 2001; Potter et al., 1998; Brown and Rosenberg, 1999; Rinaldi, 2001; Apezteguía et al., 2002), to the best of our knowledge, no similar attempts have been reported to quantify the uncertainty aspects of its predictions.

The objectives of this study were: (1) to incorporate uncertainty analysis on EPIC v3060 predictions of crop yield and SOC using the GLUE procedure, (2) to conduct sensitivity analysis using the extended FAST to identify the main sources of uncertainty in the EPIC predictions, and (3) to develop an automatic parameter optimization procedure to provide optimal parameter estimates for a study site.

MATERIALS AND METHODS

DESCRIPTION OF THE STUDY SITE

The weather, soil, and management data used in this study were from a long-term experiment conducted at the University of Wisconsin Arlington Agricultural Research Station in south central Wisconsin (43° 18′ N, 89° 21′ W) (Vanotti et al., 1997). The long-term study was established in 1958 with the purpose of evaluating the response of continuous corn (*Zea mays* L.) to N fertilization treatments. The study site lies on an extended plain with 1% to 2% slope in a Plano silt loam soil (fine-silty, mixed, mesic, Typic Argiudoll) under a humid continental climate with mean annual precipitation 791 mm and mean daily temperature 7.6°C. The responses of continuous corn to N fertilization were evaluated using a randomized complete block design with three levels of N. The block was divided into three plots (60 × 12 m) based on N fertilization rates at 0, 56, 112 kg N ha^{-1} from 1958 to 1962; at 0, 92, 184 kg N ha^{-1} from 1963 to 1972; and at 0, 140, 280 kg N ha^{-1} from 1973 to 1983 (table 1) (Vanotti et al., 1997). In 1984, each of the non-control plots was split into two subplots to study the residual effects of previous N treatments. In 1985, each subplot was further subdivided into two to evaluate the lime effects on corn yield. Because the liming period is short, only the five treatments without liming were used in this study. Fertilization rates were reduced to 0, 84, and 168 kg N ha^{-1} from 1984 till 1991 (table 1). Fertilizer N was applied about 10 days prior to planting. N was also applied to all plots as starter fertilizer during planting. The starter fertilizer was drilled 5 cm below and 5 cm to the side of the seed at the rates of 8 kg N ha^{-1} for treatment 1, 15 kg N ha^{-1} for treatments 3 and 7, and 21 kg N ha^{-1} for treatments 5 and 9 from 1958 to 1962, and then 13 kg N ha^{-1} for all plots since 1963. A detailed description of the study site can be found in Vanotti et al. (1997).

Corn yields were measured at 15.5% moisture content during 1958-1962 and 1968-1991. Corn yields of 1963-1967 were not collected but were patched based on yields in 1958-1962 and 1968-1983 (M. B. Vanotti, personal communication). For this analysis, corn yields are expressed on a dry basis. SOC content in the top 0.2 m was measured in the initial year 1958, and then in 1984 and 1990. The SOC data of 1984 and 1990 were used to evaluate the model performance in simulating SOC dynamics.

Table 1. N fertilization treatments.

Year	Fertilizer	N Fertilization Rate (kg N ha^{-1})				
		Treatment 1[a]	Treatment 3	Treatment 7	Treatment 5	Treatment 9
1958-1962	Ammonium nitrate	0	56		112	
1963-1972	Anhydrous ammonia	0	92		184	
1973-1983	Anhydrous ammonia	0	140		280	
1984-1991	Urea	0	0	84	0	168

[a] Control plot.

DESCRIPTION OF EPIC AND INPUT DATA

EPIC was originally developed in the early 1980s to simulate the impacts of soil erosion on soil productivity in the U.S. (Williams et al., 1984, Williams, 1995). It has since evolved into a comprehensive agro-ecosystem model to include the major soil and water processes related to crop growth and environmental effects of farming activities, and it continues to be modified and refined. More recent versions of this model include the improved carbon and nitrogen algorithms to estimate soil carbon sequestration (Izaurralde et al., 2001a) based on concepts and equations from the Century model as described by Parton et al. (1987, 1994) and Gassman et al. (2004).

The major components in EPIC are weather simulation, hydrology, erosion-sedimentation, nutrient cycling, pesticide fate, plant growth, soil temperature, tillage, economics, and plant environment control (Williams, 1995). It is a field-scale model that simulates processes extending only to the bottom of the root zone and edge of the field. EPIC operates on a daily time step. The number of output variables is large. The concerns in this study were crop yield and SOC predictions.

The plant growth model in EPIC is capable of simulating agronomic crops, pastures, and trees, with each crop having unique values for the model parameters, e.g., harvest index (HI), potential heat units (PHU), and maximum leaf area index (LAI). Plant growth is simulated with a heat unit system that correlates plant growth with temperature. Potential crop growth and yield are usually not achieved because of constraints imposed by the plant environment, such as water, nutrient, temperature, or aeration stresses. The root growth constraint is the minimum of soil strength, temperature, and aluminum toxicity. Crop yield may be reduced through water-stress-induced reductions in the harvest index.

Nutrient cycles are modeled in EPIC for fractions of carbon (C), nitrogen (N), and phosphorus (P). The fractions are subdivided into pools. Transformations between the different pools are calculated on a daily time step through a series of coupled equations that are solved within a mass balance framework. These equations are closely tied to other model components, including the hydrology component, which controls most of the transport processes, and the plant growth component, which handles nutrient uptake. As in the Century model, C and N compounds in EPIC are allocated to biomass, slow, and passive pools. Detailed descriptions of the EPIC components and the mathematic relationships used to simulate the processes can be found in Williams (1995). More detailed information on historical EPIC development can be found in Gassman et al. (2004).

EPIC requires the user to input weather, soil, field management, and site information. The daily on-site weather data (precipitation, maximum and minimum temperature, solar radiation, relative humidity, and wind speed) were measured for the 34-year (1958-1991) study period. The historical daily weather data were directly used in the EPIC simulation. The soil profile was divided into five layers. EPIC requires layer depth, bulk density (BD), wilting point (WP), field capacity (FC), percentage sand and silt, pH, and percentage organic C. Table 2 lists the layer data for the 1.83 m Plano silt loam soil. The data were primarily based on measured values in 1958. Soil bulk density inputs for the upper 0.36 m were mean values measured at depth intervals of 0.0 to 0.2 m and 0.2 to 0.3 m. Soil water contents at field capacity and wilting point were 0.33 and 0.18 m m^{-1} for the 0.0 to 0.3 m depth, 0.34 and 0.2 m m^{-1} for the 0.3 to 0.6 m depth, and 0.35 and 0.22 m m^{-1} for the 0.6 to 0.9 m depth. Soil pH was 6.75 for the upper 0.36 m, and the percentage soil organic C was 1.88% measured in the top 0.2 m. The remaining soil layer properties were determined based on the Plano soil data retrieved from Soil Survey Geographic (SSURGO) database.

The field management is summarized in table 3. All five treatments had the exactly same tillage operations and planting/harvesting dates. N fertilization rates were the only difference. Fertilizer N was applied 10 days prior to planting in 26 out of 34 years. In other years, N was applied about 10 days prior to planting. N was also applied as starter fertilizer during planting. Corn was planted every year, usually between the 1st and 4th weeks of May and usually harvested in the 4th week of October. Crop residues were plowed into the soil the following spring. Other required parameters, such as crop parameters, fertilizer parameters, tillage operation parameters, and other miscellaneous parameters, were set to standard values contained in EPIC parameter data files, except for the parameters chosen for uncertainty analysis listed in table 4 (see the following section). Several methods can be used to estimate runoff and potential evapotranspiration in EPIC. For this study, runoff was estimated using the USDA-SCS runoff curve number method (Mockus, 1972) with modifications incorporated for slope and soil profile water distribution effects as described by Williams (1995), and potential evapotranspiration using the Penman-Monteith method (Monteith, 1965).

Table 2. Properties by layer for the Plano silt loam soil.

Property	Soil Layer				
	1	2	3	4	5
Depth (m)	0.20	0.36	1.24	1.52	1.83
BD (Mg m^{-3})	1.47	1.49	1.49	1.55	1.53
WP (m m^{-1})	0.18	0.18	0.21	0.14	0.09
FC (m m^{-1})	0.33	0.33	0.35	0.30	0.27
Sand (%)	9.5	9.5	6.9	32.9	14.0
Silt (%)	68.0	68.0	63.1	43.6	71.0
Soil pH	6.75	6.75	6.20	6.45	7.00
Organic C (%)	1.88	1.70	0.35	0.17	0.17

Table 3. Summary of management activities for the 34-year study period (1958-1991).

Date	Management Activity
9 April - 14 April	Tillage
About 10 days before corn planting	Fertilizer application
22 April - 29 May	Tillage
24 April - 31 May	Corn planting, and starter fertilizer application
2 October - 25 October	Corn harvest

Uncertainty and Sensitivity Analyses Procedure for Evaluating EPIC

Parameter Selection

The uncertainty and sensitivity analyses were performed for two EPIC components: crop growth and SOC. In theory, the components contain a large number of input parameters. Ideally, all parameters should be treated stochastically and included in uncertainty analysis; however, this would result in an unrealistically high number of simulations, and the related computational load might be impractical (Thorsen et al., 2001). Therefore, the input uncertainty was limited to six yield-related and three SOC-related key parameters (table 4), which were selected by experience (J. R. Williams and T. J. Gerik, personal communication) to be known as the key parameters in the processes governing the plant growth and carbon dynamics. Recognizing uncertainty from only a few parameters is a more practical and typical manner in which to conduct uncertainty analysis; for instance, five parameters were chosen for uncertainty assessment in the coupled MIKE SHE/DAISY modeling system in Thorsen et al. (2001), and four parameters were chosen for uncertainty estimation in the IHDM (Institute of Hydrology Distributed Model) modeling in Beven and Binley (1992).

The biomass to energy ratio (WA) is the crop parameter for converting solar energy into biomass. The harvest index (HI) is the ratio of economic yield to the above-ground biomass. The potential heat units (PHU) is the number of heat units expected for a typical growing season (from planting date to harvest date) for the crop to mature. Heat units are accumulated degrees of temperature (°C) between the day's mean temperature and the crop's minimum growth temperature. The water stress-harvest index, PARM(3), sets the fraction of growing season when water stress starts to reduce the HI. The SCS curve number index coefficient, PARM(42), regulates the effect of potential evapotranspiration in driving the SCS curve number retention parameter. The retention parameter impacts runoff volume and changes with soil water content. The differences of soil water contents for each layer between field capacity and wilting point (DIFFW) impact water storage for plant use and water stress factor for crop growth. FBM is the fraction of organic C present as microbial biomass (active pool) at the initiation of the study. The fraction of humus in the passive C pool (FHP) is also set at the beginning of the simulation. These two thus define the distribution of the soil C pools (i.e., active or microbial, slow, and passive). The microbial decay rate coefficient, PARM(20), impacts C mineralization.

The triangular distribution was assumed for all the nine selected parameters based on expert judgment (J. R. Williams, personal communication), due to the following reasons: (1) it is difficult to determine the actual form of the probability distribution function (PDF) since it is generally not possible to collect a large, random sample to test various PDFs for their ability to describe the uncertainty in parameters (Haan et al., 1998; Beven and Binley, 1992); (2) knowledge of the means and variances of the input parameters is far more important than knowledge of the exact PDFs based on the study conducted by Haan et al. (1998); and (3) the generalized likelihood uncertainty estimation (GLUE) (Beven and Binley, 1992; Beven, 1993) was used for uncertainty analysis in this study. In the GLUE procedure, model responses are compared with observations and each parameter set is weighted via the likelihood measures; the new distribution should dominate the prior distribution when uncertainty estimates are calculated based on the likelihood weights (Beven and Binley, 1992). The means of WA and HI were taken from the default crop parameter values for corn. The means of DIFFW were based on the analysis of available data. The means of PARM(3) and PARM(42) were the values recommended for EPIC v3060 in the model documentation (www.public.iastate.edu/~elvis/i_epic_table_parameters.html). The means of the other parameters were based on expert knowledge (J. R. Williams, personal communication). The ranges for the nine selected parameters were based partly on the literature and partly on expert knowledge, as listed in table 4. Bouman (1994) stated that the ranges of the parameter values should be as broad as possible, as long as they are not beyond

Table 4. EPIC parameters used for uncertainty and sensitivity analysis.

Parameter	Symbol	Triangular Distribution		Source of Range
		Mean	Range	
Yield related				
Biomass-energy ratio (kg ha^{-1} MJ^{-1} m^2)	WA	40	30 - 45	Sinclair and Muchow (1999) and Gerik (personal communication)
Harvest index	HI	0.5	0.45 - 0.60	Kiniry et al. (1997) and Gerik (personal communication)
Potential heat units (°C)	PHU	1500	1200 - 2400	Gerik (personal communication)
Water stress-harvest index	PARM(3)	0.5	0.3 - 0.7	Williams (personal communication)
SCS curve number index coefficient	PARM(42)	1.5	0.5 - 2	Williams (personal communication)
Difference of soil water contents at field capacity and wilting point (m m^{-1})	DIFFW	0.13	0.05 - 0.2	Morgan et al. (2003) and Williams (personal communication)
Soil organic C related				
Fraction of organic carbon in microbial biomass pool	FBM	0.04	0.005 - 0.06	Williams (personal communication)
Fraction of humus in passive pool	FHP	0.7	0.3 - 0.9	Williams (personal communication)
Microbial decay rate coefficient	PARM(20)	0.1	0.05 - 1.5	Williams (personal communication)

the validity domain of the model. Although the determination of the actual form of the distributions, means, and ranges to assign to the selected input parameters seems rather subjective, it was hard to find a better way of doing this in the case of lacking data.

Uncertainty Analysis

The GLUE procedure was used for uncertainty analysis. A thorough description of the GLUE procedure can be found in Beven and Binley (1992) and Beven (1993). The procedure is based on making a large number of simulations of a given model with different sets of parameter values, chosen randomly from specified distributions. Based on comparing the predicted and observed values for each simulation, each set of parameter values was assigned a likelihood indicating the goodness of fit of model performance. Among the different possible likelihood measures (Beven and Binley, 1992; Romanowicz et al., 2000; Ratto et al., 2001), the following was used in this study for calculating the likelihood (L) of the model run corresponding to the ith set of parameters (θ_i):

$$L(\theta_i \mid O) = \exp\left(-\frac{MSE_i}{\min(MSE)}\right), \; (i = 1, 2, 3, ..., N) \qquad (1)$$

where O is the observation vector (O_1, O_2, ..., O_T), N is the total number of simulations, MSE_i is the mean squared error for the ith model run, and min(MSE) is the minimum MSE among the N simulations corresponding to the N sets of parameters. MSE_i was calculated as:

$$MSE_i = \frac{1}{T}\sum_{t=1}^{T}(P_t(i) - O_t)^2 \qquad (2)$$

where T is the number of time points for which observations are available, and P_t and O_t are the predicted and observed values for the same time point t, respectively. The likelihood measures were weighted using:

$$L_w(\theta_i) = \frac{L(\theta_i \mid O)}{\sum_{i=1}^{N} L(\theta_i \mid O)} \qquad (3)$$

where $L_w(\theta_i)$ is the likelihood weight for the ith set of parameters (θ_i). The rescaled likelihood measures have a sum of 1:

$$\sum_{i=1}^{N} L_w(\theta_i) = 1 \qquad (4)$$

which yields a relative probability of acceptability scale for the parameter sets. The uncertainty estimation was performed by calculating the model output cumulative distribution together with prediction quantiles based on the likelihood weights. Assuming that the confidence intervals (CI) are symmetrical with respect to probability, the 90% CI can be found by reading the 5% and 95% quantiles from the empirical cumulative probability plot (Haan and Skaggs, 2003a). The use of a likelihood weight allows conditioning of the model output to observations, without changing the sample and without making further model runs. A limitation of the procedure is that the observations used to compare with the predictions are assumed to be correct.

The applied sampling strategy for the GLUE analysis in this study was designed also for the computation of variance-based sensitivity indices; therefore, by applying the same set of model runs, predictive uncertainty was estimated, and sensitivity indices were calculated, too. For this purpose, a Sobol sample (Sobol, 1993) or the extended Fourier amplitude sensitivity test (FAST) sample (Saltelli et al., 1999) should be used. The extended FAST sample was used in this study since it has the advantage of a small sample size in comparison to the method of Sobol (Schwieger, 2004; Saltelli et al., 1999). Since the GLUE procedure considers that each model realization is associated with a particular set of parameters rather than individual parameter values, in order to reduce the noise from unrelated parameters for specific model component, the yield-related and SOC-related parameter sets were generated separately while running the model with the unrelated parameter values fixed using base values. The base values are the parameter means given in table 4, except FBM using the observed 0.01 and FHP using the default 0, which sets the model to calculate it automatically according to the number of years that the soil is under cultivation. A total of 1,500 parameter sets were generated for each of the two components using the public domain SIMLAB software (2003) from the given ranges and distribution specified in table 4. SIMLAB provides an interface for sample generation designed for uncertainty and sensitivity analyses of model outputs. The extended FAST sampling method designed for all total and first-order effect calculation was used. The EPIC source code was modified for parameter update using the generated parameter sets. For each of the generated parameter sets, the EPIC model was run continuously for all years (1958-1991). The EPIC runs were then evaluated using likelihood measure (eq. 1) and weighted using equation 3 in GLUEWIN (2003), a Windows program designed for uncertainty analysis using the GLUE procedure (Ratto and Saltelli, 2001). The likelihood weights were used as the basis for the uncertainty analysis. Predicted mean values over the 1,500 runs, variances, probability distributions, cumulative density distributions, together with 90% CIs were used to characterize prediction uncertainty.

Variance-Based Sensitivity Analysis

A complete and detailed description of variance-based sensitivity analysis can be found in Saltelli et al. (2000). Variance-based sensitivity analysis is based on generated samples. After the model executions using the generated samples, the output variance is analyzed, and the sensitivity analysis is based on analyzing the output variance in relation to the variation of the input quantities (Schwieger, 2004).

The first-order sensitivity index (S_i) represents the sensitivity of prediction (P) or likelihood weight (L_w) to singular parameter (X_i) (Schwieger, 2004; Ratto et al., 2001), given by:

$$S_i(P) = \frac{V(E(P \mid X_i = x_i^*))}{V(P)} \qquad (5)$$

$$S_i(L_w) = \frac{V(E(L_w \mid X_i = x_i^*))}{V(L_w)} \qquad (6)$$

where $V(P)$ is the total variance of predictions; $V(L_w)$ is the total variance of likelihood weights; $V(E(P \mid X_i = x_i^*))$ is the conditional variance of $E(P \mid X_i = x_i^*)$, which is the expectation of P conditional on X_i known and having a fixed value x_i^*; and $V(E(L_w \mid X_i = x_i^*))$ is the conditional variance of $E(L_w \mid X_i = x_i^*)$, which is the expectation of L_w conditional on X_i known and having a fixed value x_i^*.

If the expectation value E varies considerably with the selection of a particular value x_i^* for X_i, while all the effects of the X_j values $(j \neq i)$ are being averaged, then surely parameter X_i is an influential one (Schwieger, 2004). The expectation value E above the whole variation interval of the input quantity X_i has to be evaluated to get a global sensitivity measure.

The computation of all higher-order terms requires high computational costs. An efficient alternative is to compute the total sensitivity index (S_{Ti}) with respect to an input quantity X_i based on all effects involving X_i. The total sensitivity index represents the overall impact of parameter X_i on prediction (P) or likelihood weight (L_w), whether the effects are additive or not, given by:

$$S_{Ti}(P) = \frac{E(V(P \mid X_{\sim i} = x_{\sim i}^*))}{V(P)} \qquad (7)$$

$$S_{Ti}(L_w) = \frac{E(V(L_w \mid X_{\sim i} = x_{\sim i}^*))}{V(L_w)} \qquad (8)$$

where $X_{\sim i}$ indicates all the parameters except X_i, $E(V(P \mid X_{\sim i} = x_{\sim i}^*))$ is the average prediction variance conditional on all input quantities ($X_{\sim i}$) apart from X_i holding fixed as values $x_{\sim i}^*$ and X_i remaining variable (Schwieger, 2004), and $E(V(L_w \mid X_{\sim i} = x_{\sim i}^*))$ is the average likelihood weight variance.

Special sampling schemes are required to estimate the pair (S_i, S_{Ti}) (Saltelli et al., 2000; Schwieger, 2004). The extended FAST (Saltelli et al., 1999) was used in this study. The method is based on Fourier transformation of uncertain model input parameters into a frequency domain, which converts a multidimensional integral over all the uncertain parameters to a one-dimensional integral, and constructs a search curve to scan the entire parameter space (Saltelli et al., 1999). A thorough description of the extended FAST sampling procedure and the efficient estimators are provided in Saltelli et al. (1999). The SIMLAB software was used to conduct the FAST sensitivity analyses based only on the model predictions (without comparing to observed values) (eqs. 5 and 7) and based on likelihood weight (eqs. 6 and 8).

Automatic Parameter Optimization Procedure

An automatic parameter optimization procedure was developed using a multi-objective function at the conclusion of the sensitivity analysis following these steps:

1. A number of 1,500 random parameter sets were generated for the most influential and uncertain parameters from the given ranges and distributions (table 4). Prabhu (1995) determined that at least 1,500 model runs must be done for representative results.
2. EPIC was run by updating parameter values using the randomly generated parameter sets.
3. Each of the 1,500 EPIC runs were evaluated for both corn yield and SOC using the following aggregated function (F_i), which combines two objective functions into one with a weight of 0.5 for each objective function:

$$F_i = \left[0.5 \times L\left(\theta_i \mid \overline{Yield}\right)^2 + 0.5 \times L\left(\theta_i \mid Soc\right)^2\right]^{1/2} \qquad (9)$$

   where $L(\theta_i \mid \overline{Yield})$ and $L(\theta_i \mid Soc)$ are the likelihood values calculated using equation 1 for corn yield and SOC, respectively, of the EPIC run corresponding to the ith set of parameters (θ_i).
4. The largest F_i among the 1,500 F_i was identified automatically. The corresponding ith set parameter values was identified as the parameter estimations for the site.

Results and Discussion

Uncertainty Analysis

The distributions of the predicted average annual corn yields per treatment over the 34-year study period appeared approximately normal (fig. 1). The 90% CI estimated from the 5% and 95% quantiles of the cumulative distribution (fig. 2) was used as the uncertainty limits of predictions (Haan and Skaggs, 2003a; Beven and Binley, 1992; Sabbagh and Fox, 1999). Observed values fell well within the 5% and 95% confidence limits (fig. 2). The width of the 90% CI bands ranged from 0.31 to 1.6 Mg ha^{-1} (fig. 2), while predicted means over the 1,500 simulations for the average annual yield per treatment ranged from 3.26 to 6.37 Mg ha^{-1}, with observations ranging from 3.28 to 6.4 Mg ha^{-1} for the five treatments (table 5). EPIC performed successfully in predicting the effects of different N application rates on the long-term average annual corn yields, as indicated by the low mean errors ranging from −0.6% to 2.6% for the five N treatments (table 5). For each treatment, the coefficient of variation (CV) of the predicted means from the 1,500 simulations using the given ranges and distribution of the six yield-related parameters (table 4) was under 10%. The close agreement between observations and the predicted means, which can be used as a measure of the model behavior (Beven and Binley, 1992), together with relatively low CV of the predictions, indicate that EPIC was dependable and accurate in predicting the average annual corn yields.

Figure 3 shows the observed and simulated 5% and 95% confidence limits of the yearly corn yields for the study period for treatment 3 as an example. Most of the observed yearly yields of the five treatments fell within the 5% and 95% confidence limits of the predictions. The width of the 90% confidence interval bands ranged from 0.44 to 5.25 Mg ha^{-1}. The predicted means of yearly yields over the 1,500 simulations ranged from 1.77 to 9.22 Mg ha^{-1}, with observed yearly corn yields ranging from 1.35 to 10.22 Mg ha^{-1} for the five treatments. The confidence bound estimation was obtained by calculating the model output cumulative distribution based on the likelihood weights of the 1,500 simulations, which considered only the uncertainties in the six crop-related parameters (table 4). The uncertainties in other parameters, input data, observations, and the model structure were not examined.

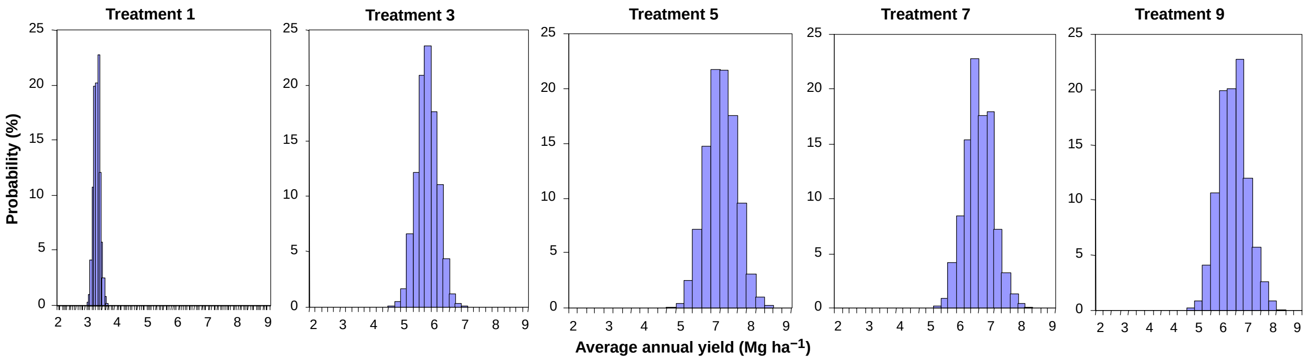

Figure 1. Probability distribution of predicted average annual corn yield over 1958-1991 for the five treatments.

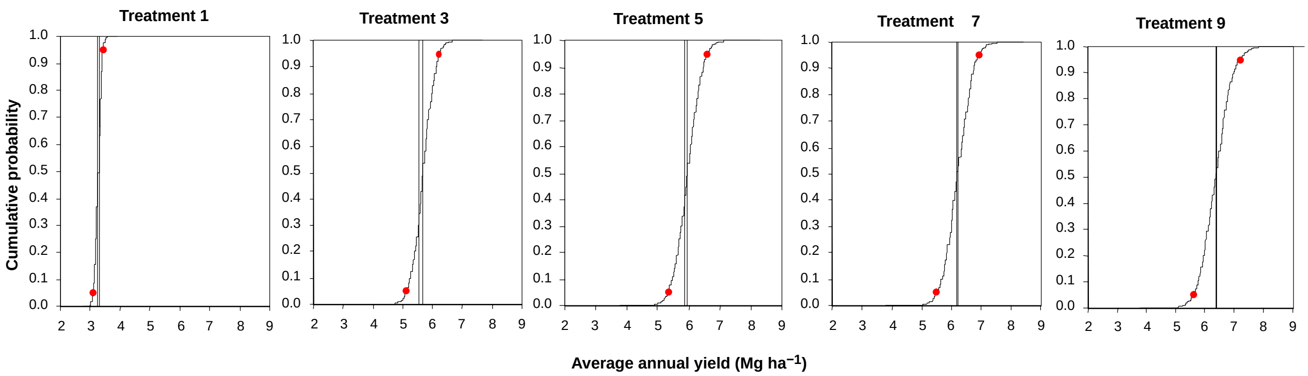

Figure 2. Cumulative distribution of predicted average annual corn yield (1958-1991) for the five treatments. The 5% and 95% quantiles are shown as dots; the mean of predictions over the 1,500 simulations is identified by a vertical solid line, while the corresponding observation is shown as a vertical dashed line.

The width of the 90% CI band of SOC in the top 0.2 m soil ranged from 285 to 625 g C m^{-2}. The predicted means of SOC for 1984 and 1990 per treatment over the 1,500 simulations ranged from 5122 to 6564 g C m^{-2}, and observations ranged from 5645 to 6733 g C m^{-2}, with the errors ranging from −9.3% to 3.3% (fig. 4). The observed SOC fell within the 5% and 95% confidence limits, except for the control treatment for both years and treatment 7 in 1990. The observed SOC in the control treatment increased from the initial year due to the return of corn residues and the low levels of initial soil organic matter as a result of prior poor management (Vanotti et al., 1997). The model simulated a decrease in SOC in the control plot. This suggests that the model might underestimate the C and N return from corn residues. It is hard to explain the poor simulation for treatment 7 in 1990. It had the highest observed SOC (fig. 4 and table 8), which is different from the observed trend where SOC decreased from 1984 to 1990 for all other treatments due to the effect of reduced N inputs in the six years. Moreover, the N fertilization rates for treatment 9 doubled those of treatment 7 for the entire experiment period, and N fertilization rate was the only difference in field operation and management. Thus, treatment 7 should not be the one with the highest SOC. Observation error is a possibility.

Table 5. Mean and standard deviation of simulated average annual corn yields (1958-1991) from the 1,500 simulations.

Treatment	Measured Annual Mean (Mg ha^{-1})	Simulated Mean (Mg ha^{-1})	SD (Mg ha^{-1})	CV (%)	Mean Error (%)
1	3.28	3.26	0.10	3.1	−0.6
3	5.54	5.69	0.33	5.8	2.6
5	5.85	5.99	0.39	6.5	2.3
7	6.17	6.22	0.43	6.9	0.8
9	6.40	6.37	0.48	7.5	−0.5

Sensitivity Analysis

Scatter plots for the likelihood weights (using eq. 3) for treatment 7 corn yield predictions versus each parameter are shown in figure 5 as an example. Scatter plots for other treatments (not shown) had similar appearances. The nonlinear shape of the scatter plots points to significant interactions among parameters. High likelihood values are distributed throughout the parameter spaces investigated. A relatively clear pattern can be identified for WA, HI, PHU, and DIFFW (fig. 5). The likelihood values significantly decrease when WA and HI increase towards the upper end of the parameter ranges, and significantly decrease when PHU and DIFFW decrease towards the lower end of the parameter ranges. No clear trend can be seen for PARM(3) and PARM(42).

The FAST sensitivity indices for sensitivity quantitative analysis based on yearly corn yields are presented in figures 6 and 7 for treatment 7 as examples. Figure 6 gives the FAST first order (singular influence of the parameter) and total order (all effects involving the parameter) sensitivity indices for chosen time series. Figure 7 gives the average sensitivity

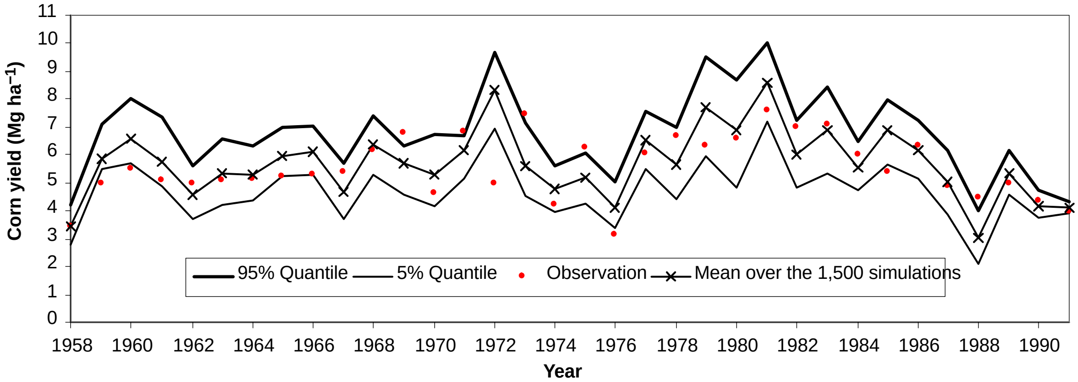

Figure 3. Simulated 5% and 95% confidence limits of yearly corn yield for treatment 3 and corresponding observations.

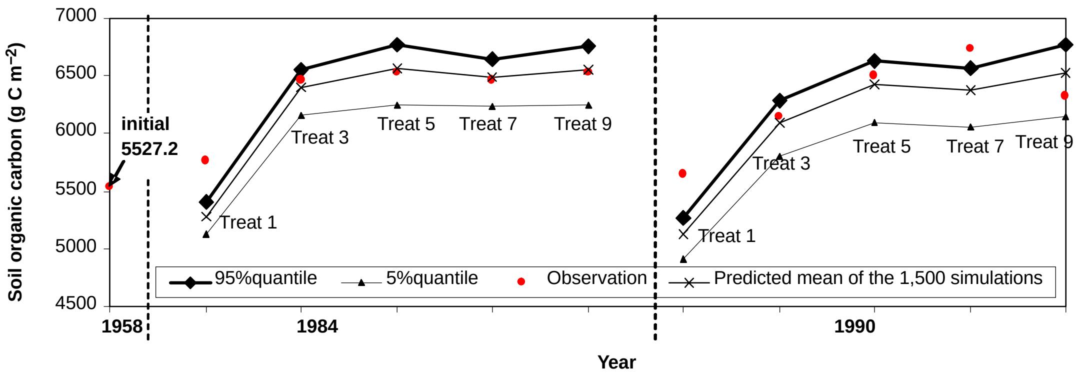

Figure 4. Simulated 5% and 95% confidence limits of SOC in the top 0.2 m soil for the five treatments and corresponding observations.

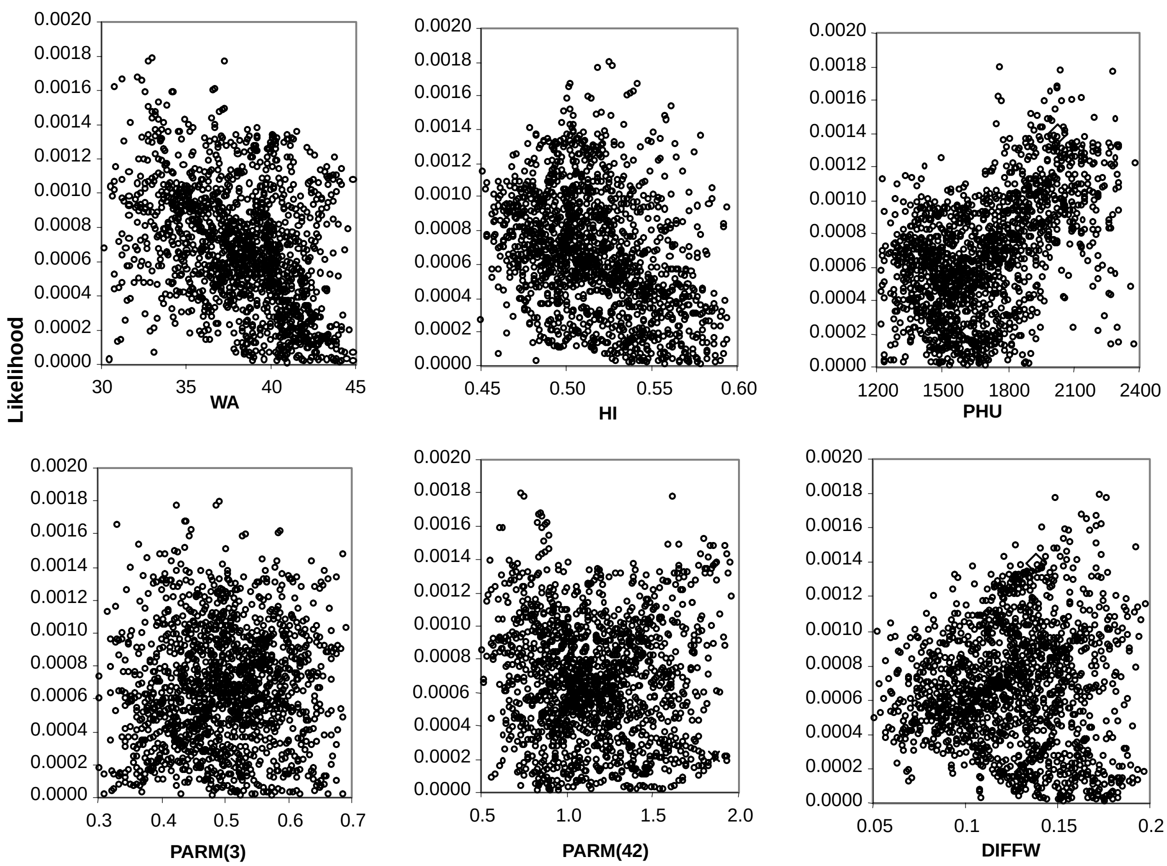

Figure 5. Scatter plots of model parameters (table 4) vs. likelihood weights of corn yield predictions for treatment 7.

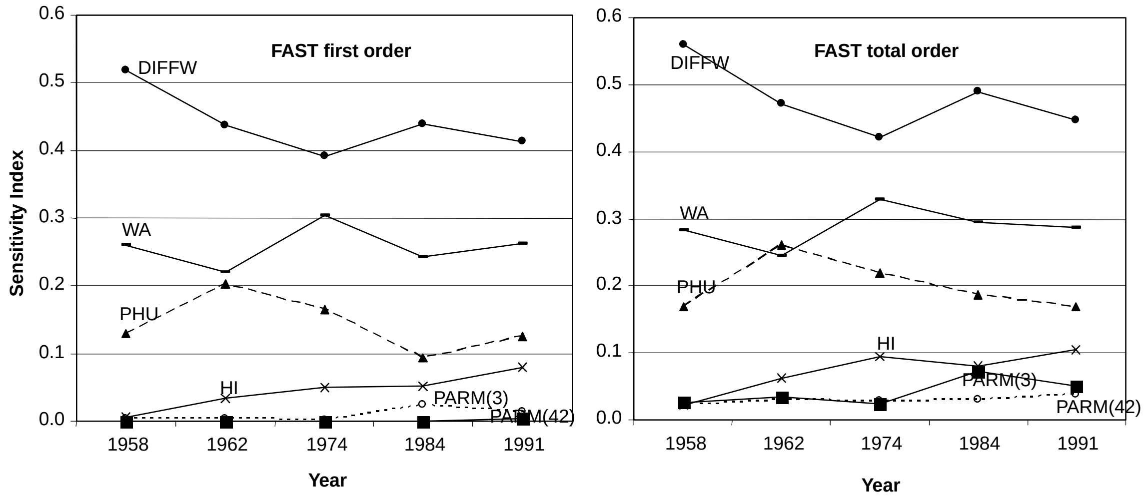

Figure 6. Sensitivity indices for yearly corn yield for treatment 7.

indices for the entire time series of 34 years. By considering the difference between the total effect sensitivity indices and the first-order sensitivity indices, a very slight increase is detected. This implies that few interactions are revealed by the analysis of the physical output, which singles out the importance of DIFFW, WA, and PHU, followed by HI.

Very high total sensitivity indices of corn yields were detected based on likelihood weights for all parameters investigated (fig. 8). This suggests that the good agreements between model predictions and observations are not driven by a particular parameter but by interactions among parameters. The increase in total-order over first-order sensitivity indices was greater when sensitivity analysis was based on likelihood values than when sensitivity analysis was based on model output alone. This reveals an advantage of using the likelihood weights, in that the effect of parameter interaction was more evident.

High total sensitivity indices of the three parameters for the EPIC SOC component based on likelihood weight were detected for all three parameters investigated (table 6 and fig. 9). Only FBM was not influential based on model output alone. Again, the increase in total-order over first-order sensitivity indices was greater when sensitivity analysis was based on likelihood weights than when sensitivity analysis was based on model output alone.

Parameter Estimation

For the EPIC crop growth component, the influential parameters are soil water capacity (DIFFW), potential heat units (PHU), biomass-energy ratio (WA), and harvest index

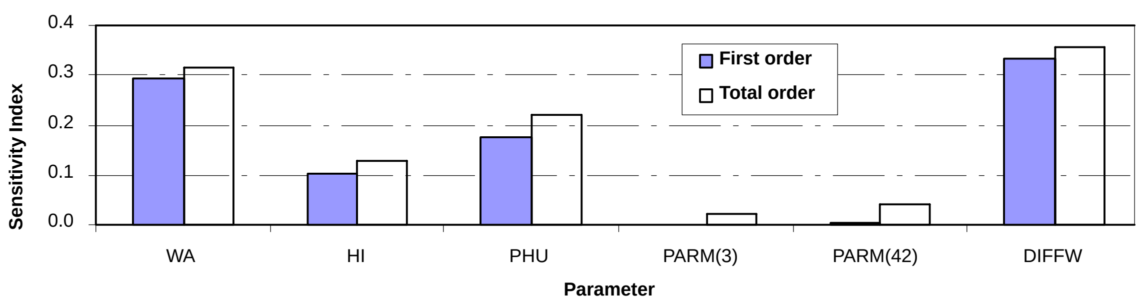

Figure 7. Sensitivity indices for yearly corn yield for treatment 7.

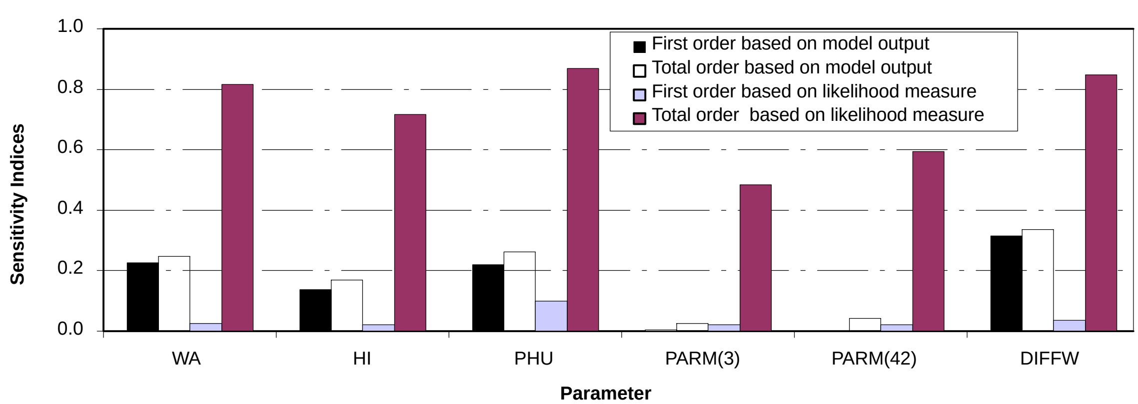

Figure 8. Sensitivity indices based on model prediction or likelihood weight for corn yield for the five treatments.

Table 6. FAST sensitivity indices for SOC.

Parameter	FBM	FHP	PARM(20)
Based on model output (before comparing to observed values)			
First order	0.0018	0.6004	0.3714
Total order	0.0117	0.6243	0.3937
Increase	0.0098	0.0239	0.0223
Based on likelihood measure (after comparing to observed values)			
First order	0.0103	0.0657	0.0911
Total order	0.5955	0.8348	0.8547
Increase	0.5853	0.7692	0.7636

(HI). Correspondingly, microbial decay rate coefficient (PARM(20)) and fraction of humus in passive pool (FHP) are critical parameters for SOC component. Since the study site had initial soil water content measurements of layers at wilting point and field capacity, those values were used. The values of the remaining five parameters were identified as 35.4 kg ha^{-1} MJ^{-1} m^2 for WA, 0.48 for HI, 1645°C for PHU, 0.86 for FHP, and 0.13 for PARM(20) based on the optimal value of the aggregated objective function (eq. 9) through the automatic parameter optimization search.

A WA of 35.4 kg ha^{-1} MJ^{-1} m^2 is similar to the values of 32 to 34 kg ha^{-1} MJ^{-1} m^2 for corn summarized by Sinclair and Muchow (1999). An HI of 0.48 is close to the values reported in many agronomic trials (Kiniry et al., 1997). A PHU of 1645°C is close to the value of 1640°C calculated using the 34-year average heat unit accumulation at the study site during the normal growing season, which was determined from May 11 to October 16 by averaging the 34 years of planting and harvest dates. An FHP of 0.86 is larger than values reported in the literature for non-hydrolyzable C, which is the extractable pool most closely associated to the passive soil organic carbon pool (Paul et al., 1997). A value of 0.13 determined for the microbial decay rate coefficient, PARM(20), was close to the mean of the triangular distribution used to parameterize the model runs. Low PARM(20) values slow down the potential transformations of the various carbon pools (i.e., structural and metabolic litter, microbial biomass, slow and passive humus).

The parameter set gives an R^2 of 0.96 with a slope of 1.1 for the average corn yield prediction and a R^2 of 0.89 with a slope of 1.3 for the yearly SOC prediction (fig. 10). The positive slopes were significantly different from zero at the 95% confidence level. Overall, the model was accurate in predicting the average annual yields and yearly SOC.

The errors for average corn yields ranged from −8.5% to 8.2% (table 7 and fig. 11). The close agreement in mean and standard deviation indicates the similarity in observed and predicted yield probability distribution. This is consistent with the finding in Williams et al. (1989) and is useful in decision making when based on model output. The errors for yearly SOC ranged from −8.3% to 2.4% (table 8 and fig. 12). This indicates that the model is reasonably acceptable for SOC prediction. However, it failed to simulate the SOC increase from the initial year for the control treatment and underestimated SOC for the treatment in both 1984 and 1990.

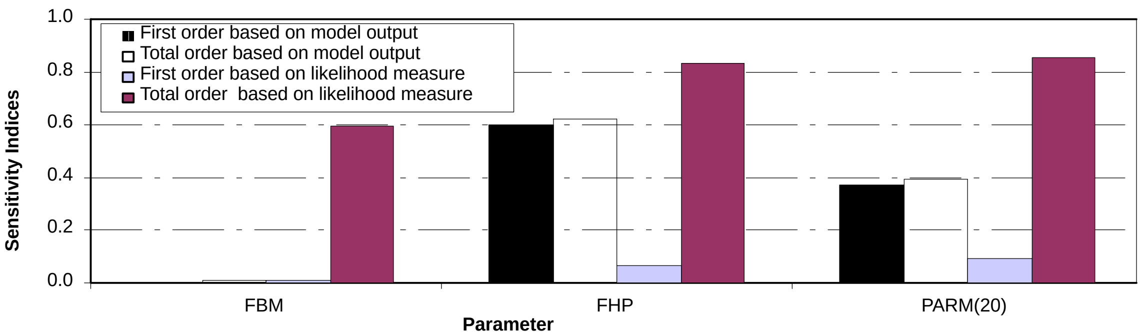

Figure 9. Sensitivity indices based on model prediction or likelihood measure of SOC for the five treatments.

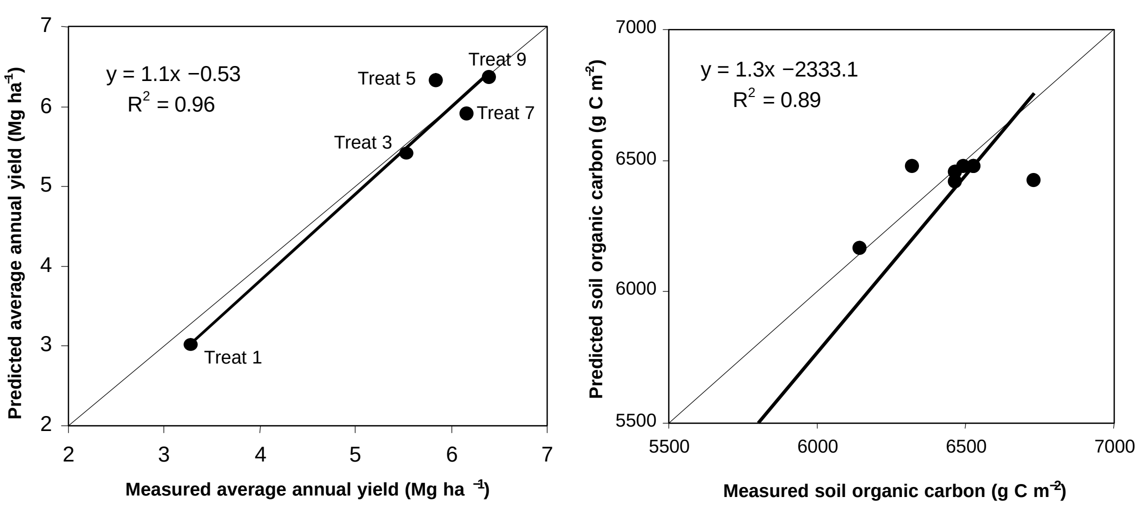

Figure 10. Measured vs. predicted mean corn yield and SOC.

As reasoned in the uncertainty analysis above, the model might underestimate the C return from corn residues. The model captured the effect of fertilizer inputs on SOC dynamics in that SOC increased significantly from the initial year 1958 to 1984 for all N treatments. On average, the observed SOC for the N treatments increased 970 g C m^{-2} from 1958 to 1984, with an average C sequestration rate of 35.9 g C m^{-2} $year^{-1}$; an increase of only 235 g C m^{-2} was observed for the control treatment for the same period of time, with an average C sequestration rate of 8.7 g C m^{-2} $year^{-1}$. On average, the predicted SOC for the N treatments increased 933 g C m^{-2} from 1958 to 1984, with an average C sequestration rate of 34.5 g C m^{-2} $year^{-1}$ (table 8). The average predicted error of C sequestration rate during 1958-1984 for the N treatments was −4%. The observed SOC decreased from 1984 to 1990 for all treatments except for treatment 7. As reasoned in the uncertainty analysis above, observation error is a possibility for treatment 7. The decrease of SOC can be attributed to the effect of reduced N fertilization for the N treatments. The model captured this decrease for the 1984 to 1990 period, too.

Table 7. Means and standard deviations of observed and predicted corn yield (1958-1991) from the optimal run.

	Observed Corn Yield				Predicted Corn Yield				
Treatment	Mean (Mg ha^{-1})	SD (Mg ha^{-1})	CV (%)	Range (Mg ha^{-1})	Mean (Mg ha^{-1})	SD (Mg ha^{-1})	CV (%)	Range (Mg ha^{-1})	Error (%)
1	3.28	1.05	31.9	1.35 - 6.42	3.00	1.03	34.2	1.04 - 5.63	−8.5
3	5.54	1.11	20.0	3.13 - 7.61	5.41	1.34	24.8	2.84 - 8.96	−2.4
5	5.85	1.26	21.5	3.46 − 7.61	6.33	1.47	23.2	2.88 - 9.06	8.2
7	6.17	1.42	23.0	3.13 - 8.96	5.90	1.23	20.9	2.88 - 8.96	−4.4
9	6.40	1.45	22.6	3.46 - 10.22	6.36	1.50	23.6	2.87 - 9.47	−0.6

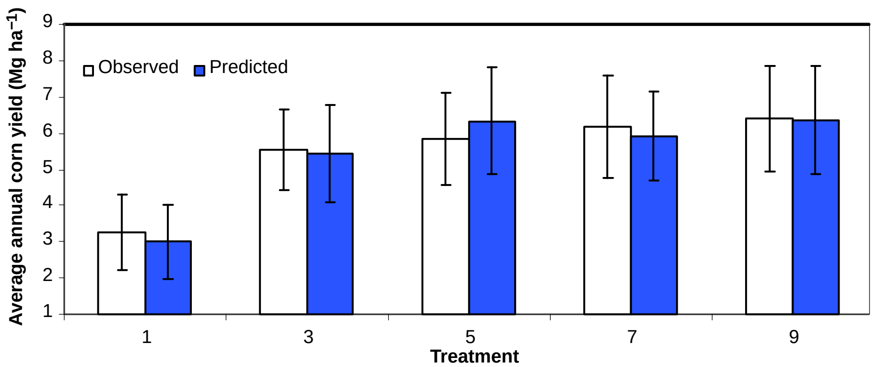

Figure 11. Measured vs. predicted average annual corn yields over 1958-1990 for the five treatments with standard error bars.

Table 8. Measured and predicted SOC of the optimal run

		SOC (g C m^{-2})			Average Annual Rate of C Change (g C m^{-2} $year^{-1}$)			
	Year	Measured	Predicted	Error (%)	1958 to 1984		1984 to 1990	
Treatment	1958 (initial)	5527.2			Measured	Predicted	Measured	Predicted
1	1984	5762.4	5303.1	−8.0	8.7	−8.3	−16.8	−18.2
	1990	5644.8	5175.7	−8.3				
3	1984	6468.0	6418.3	−0.8	34.9	33.0	−46.2	−36.0
	1990	6144.6	6166.2	0.4				
5	1984	6526.8	6477.4	−0.8	37.0	35.2	−4.2	−0.2
	1990	6497.4	6476.0	−0.3				
7	1984	6468.0	6458.4	−0.1	34.9	34.5	37.8	−5.2
	1990	6732.6	6422.0	−4.6				
9	1984	6526.8	6477.4	−0.8	37.0	35.2	−29.4	−0.3
	1990	6321.0	6475.2	2.4				

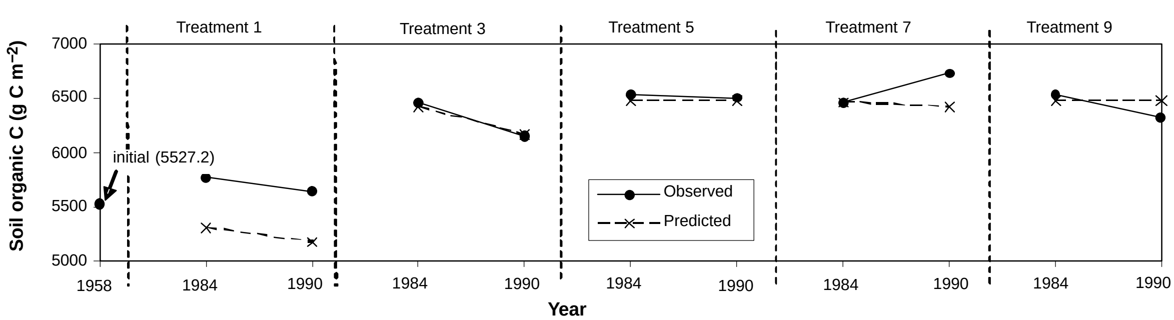

Figure 12. Measured vs. predicted SOC for the five treatments.

Conclusions

Uncertainty and sensitivity analyses were performed for corn yields and SOC dynamics simulated with the EPIC model using data from the Arlington Agricultural Research Station in Wisconsin. The GLUE procedure was used to obtain output probability distribution functions and confidence limits based on likelihood weights. The uncertainty estimations were only based on six crop-related parameters and three SOC-related parameters; other error sources were not examined in this study. Results show that the observed average corn yields fell well within the 5% and 95% confidence limits for all treatments, suggesting that EPIC was dependable and accurate, from a statistical point of view, in predicting average annual corn yield. The observed yearly SOC fell within the confidence limits ,except for the control treatment and treatment 7 in 1990, with mean errors ranging from −9.3% to 3.3%. The results also revealed possible error sources, such as error in observations and model structural error in underestimating the return of corn residues.

The GLUE procedure allows the performance of sensitivity analysis based on likelihood weights. When the FAST sensitivity analysis was based on model prediction alone, it only identified the individual influence of available soil water capacity (DIFFW), potential heat units (PHU), biomass-energy ratio (WA), and harvest index (HI) for the crop growth component, and microbial decay rate coefficient (PARM(20)) and fraction of humus in passive pool (FHP) for the SOC component. Few interactions among parameters were revealed. However, when the sensitivity analysis was based on likelihood weights, it revealed more interaction influence, meaning that good results are not driven by a particular parameter but by a set of interactive parameters.

An automatic parameter optimization procedure was developed in this study, which identified the optimal parameter set for the most influential and uncertain parameters for the study site based on a multi-objective function value. The model did a good job in predicting corn yield and SOC using the optimal parameter set, with R^2 of 0.96 for average annual corn yield predictions and 0.89 for yearly SOC.

The study demonstrated a widely applicable procedure of combining the GLUE procedure and a variance-based sensitivity analysis technique with an agronomic model for evaluating the prediction uncertainty associated with uncertain parameters, together with an automatic parameter optimization procedure on the basis of sensitivity analysis and the use of a multi-objective function. The procedure is efficient in that the use of a likelihood weight allows conditioning model output to observations, without changing the sample and without making further model runs. By applying the same set of model runs, prediction uncertainty was estimated and sensitivity indices were calculated, too. Modelers or policymakers can use the procedure for any deterministic models of their interest. Because of the use of likelihood weight in the procedure, potential model users may apply the parameter ranges proposed in this study to different soils and climate if data are not available. The limitation of the procedure is that the uncertainties in model structure and observations were not examined. This should be the focus of future study. For example, by comparing EPIC with other models using the same procedure and observations, the uncertainties in the model structure can be explored. Opportunity also exists for improvement in the procedure to include a parameter screening step to identify the key parameters for the further uncertainty and more complex sensitivity analyses.

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